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Maximum entropy principle for rarefied polyatomic gases

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ABSTRACT

The aim of this paper is to show that the procedure of maximum entropy principle for the closure of the moments equations for rarefied monatomic gases can be extended also to polyatomic gases. The main difference with respect to the usual procedure is the existence of two hierarchies of macroscopic equations for moments of suitable distribution function, in which the internal energy of a molecule is taken into account. The field equations for 14 moments of the distribution function, which include dynamic pressure, are derived. The entropy and the entropy flux are shown to be a generalization of the ones for classical Grad's distribution. The results are in perfect agreement with the recent macroscopic approach of extended thermodynamics for real gases.

1. Introduction

The aim of this paper is to establish a macroscopic model for non-equilibrium processes in rarefied polyatomic gases using the approach of the maximum entropy principle (MEP). To reach that goal we use the kinetic model proposed by Bourgat, Desvillettes, Le Tallec and Perthame [1], in which the distribution function depends on an additional continuous variable that takes into account the internal energy of a molecule.

The entropy maximization, which has its roots in statistical mechanics and information theory, proved to be successful in the case of monatomic gases. Namely, it was shown (see Ref. [2]) that in the case of 13 fields the following three procedures yield the same macroscopic equations for monatomic gases: (i) Grad's moment method, (ii) extended thermodynamics (ET) of viscous, heat-conducting gases and (iii) maximization of entropy. An interesting review on irreversible thermodynamics, which also elucidates different pathways to macroscopic equations, is recently given by Müller and Weiss [3].

The closure problem for suitable set of macroscopic equations is at the heart of the issue and each of these procedures is aimed at solving it. The Grad's moment method is focused on finding the approximate non-equilibrium velocity distribution function $f(t, \mathbf{x}, \boldsymbol{\xi})$ which closes the system of balance laws in the physical case of 13 moments. The celebrated solution, given by Grad [4], is based upon expansion of distribution function in terms of tensorial Hermite polynomials. This procedure led to the system of balance laws for 13 moments of f, i.e. fields of mass density, velocity, temperature, stress tensor and heat flux.

The extended thermodynamics (ET) [2,5], as primarily macroscopic theory, arrived at the same set of equations by imposing universal principles of relativity, entropy inequality with convex entropy. Motivated by the similarity of ET and moment equations derived from the Boltzmann equation on one hand, and Kogan's observation that Grad's distribution function maximizes the entropy [6] on the other, a maximum entropy principle was established first by Dreyer [7]. In the first

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edition of the book of ET of Müller and Ruggeri [8], this procedure was extended for any number of moments. Successively, a similar result was given by Levermore [9]. The complete equivalence between entropy principle and MEP was subsequently proved by Boillat and Ruggeri [10].

The success in the study of monatomic gases by the methods previously described has not been achieved in the case of polyatomic gases. The inclusion of new degrees of freedom (rotation and vibration) enriched the physical insight at the expense of mathematical coherence of the procedure [11]. In particular, internal energy density is no longer related to the trace of the second moment of distribution function, which prevents construction of simple hierarchy of transfer equations for moments. Moreover, complex physical description made solution procedures extremely complicated even for slightly involved problems.

Concerning the kinetic approach, a new light was shed on the problem when the model for binary collisions was introduced by Borgnakke and Larsen [12], which takes into account an exchange of energy (other than translational) during the collision. It was initially used for Monte Carlo simulations of polyatomic gases, but also applied for derivation of appropriate Boltzmann equation [1].

In the macroscopic framework, an ET theory for real gases has been successfully developed only very recently by Arima, Taniguchi, Ruggeri and Sugiyama [13], after several pioneering papers [14,15]. This is the theory of 14 fields of mass density, velocity, temperature, viscous stress, dynamic pressure, and heat flux with two parallel hierarchical series of field equations of balance type. The constitutive equations are determined explicitly by the thermal and caloric equations of state. The theory naturally includes the special case of rarefied polyatomic gases and, as a singular limit, the case of monatomic gases. This approach was applied also for derivation of 6 moments ET model which extends the Meixner's theory [16].

Our aim is to show that the maximum entropy principle applied to the kinetic model for polyatomic gases yields appropriate macroscopic balance laws for 14 independent fields, and presents a natural generalization of the same procedure applied for monatomic gases. The principal novelty, which is in accordance with the conjecture of ET of real gases [13], is that we obtain two hierarchies of transfer equations for moments, in contrast to one hierarchy in the case of monatomic gases. One of them is related to classical moments of distribution function, i.e. "*momentum-like*" moments. Another independent hierarchy, which starts with the second order moment corresponding to internal energy density, is expanded into transfer equations for "*energy-like*" moments. This hierarchy, however, cannot be merged into the first one since internal energy density is no longer twice the trace of the classical second order moment, as it is in monatomic case.

The paper is organized as follows. The Section 2 contains a brief review of classical results related to the application of the maximum entropy principle in kinetic theory of monatomic gases. In Section 3 the basic features of the model for polyatomic gases will be discussed at the Euler level. In particular, an equilibrium distribution function will be derived using maximum entropy principle, coinciding with the equilibrium distribution deduced in Ref. [1] by means of the H-theorem, with accompanying Euler equations. This will also be the preparatory material for the next two sections where new non-equilibrium results will be given. Namely, Section 4 will contain an exposition of the main idea of the paper—to construct two independent hierarchies of moment equations, "momentum" and "energy" ones.

The Section 5 will be focused on 14 moments approximation of the velocity distribution function. First, the non-equilibrium velocity distribution function will be derived by means of the maximum entropy principle, which will permit explicit derivation of the non-convective fluxes. Moreover, the entropy density and entropy flux will be determined for polyatomic gases, both in equilibrium and non-equilibrium case. It will be shown that Gibbs' relation holds for equilibrium distribution function, whereas entropy density and entropy flux represent generalization of the Grad's ones, since they comprise the dynamic pressure. Then the corresponding set of balance laws (field equations) as transfer equations for moments will be derived in the spirit of procedure described in Section 4. The results obtained are in complete agreement with the ones of ET of polyatomic gases, which leads to the conclusion that the entropy principle of ET is equivalent to MEP in the case of rarefied polyatomic gases.

Finally, we evaluate the explicit expression of production terms, relaxation times and phenomenological parameters (viscosity coefficients and heat conductivity) using a simple collision model.

The section finishes with discussion on the qualitative analysis in the framework of symmetric hyperbolic systems. At the end, some remarks about further problems will be given.

2. Moment equations and entropy maximization

The kinetic theory of gases assumes that the state of the monatomic gas is described by the velocity distribution function $f(t, \mathbf{x}, \boldsymbol{\xi})$. Then $f(t, \mathbf{x}, \boldsymbol{\xi})\, \mathrm{d}\mathbf{x}\, \mathrm{d}\boldsymbol{\xi}$ is the number of atoms in the volume $\mathrm{d}\mathbf{x}\, \mathrm{d}\boldsymbol{\xi}$ of phase space centered at $(\mathbf{x}, \boldsymbol{\xi}) \in \mathbb{R}^3 \times \mathbb{R}^3$. The time rate of change of the velocity distribution function in the absence of external forces is determined by the Boltzmann equation

$$\partial_t f + \xi_j \partial_j f = Q(f), \tag{1}$$

where the collision integral $Q(f)$ determines the collision rate of change of distribution function. The symbols ∂_t and ∂_j denote partial derivatives with respect to time t and space variables x_j, respectively.[1] Finding a solution of (1) is an extremely

[1] Throughout the paper summation with respect to repeated indices will be assumed.